COMPONENTS:

- (1) Butane; C₄H₁₀; [106-97-8]
- (2) Water; H_2O ; [7732-18-5], at high pressure

EVALUATOR:

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December 1983

CRITICAL EVALUATION:

There are four studies of this system at high temperatures and pressures. The data of Tsiklis and Maslennikova (1) are rejected since they are restricted to the critical region and are in serious disagreement with the data of Danniel $et\ al.$ (2). Furthermore they appear to be anomalous when the data for alkane + water systems are considered. Therefore the data of Tsiklis and Maslennikova (1) are rejected. The limited data of Danniel $et\ al.$ (2) are classified as tentative on the basis that they appear consistent with data in the critical region of other workers for alkane + water mixtures.

There are significant discrepancies between the data of Reamer $et\ al.$ (3) and Le Breton and McKetta (4). The latter data are probably the more reliable and are classified as tentative. The temperature range studied in references (1) and (2) does not overlap with the range studied in references (3) and (4).

References

- Tsiklis, D. S.; Maslennikova, V. Ya.
 Dokl. Akad. Nauk. S.S.S.R. 1964, 157, 426.
- Danniel, A.; Tödheide, K.; Franck, E. U.
 Chem.-Ing.-Tech. 1967, 39, 816.
- Reamer, H. H.; Sage, B. H.; Lacey, W. N.
 Ind. Eng. Chem. 1952, 44, 609.
- 4. Le Breton, J. C.; McKetta, J. J.

 Hydroc. Proc. Pet. Ref. 1964, 43 (6), 136.

COMPONENTS:

- (1) Butane; C₄H₁₀; [106-97-8]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Le Breton, J.G.; McKetta, J.J.

Hydroc. Proc. Pet. Ref. 1964, 43, 136-138.

VARIABLES:

T/K: 310.9-410.9 P/kPa: 129.3-3044

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t¹/°F	T 2/K	Total Pressure ¹ /psia	Partial Pressure ² P/kPa	Mol Fraction $10^5 x_{\tilde{I}}$
				
100	310.9	19.7	129.3	1.73
		23.7	156.9	1.92
		29.7	198.2	2.78
		34.7	232.7	2.92
		41.2	277.5	3.76
		52.2	353.4	$(4.61)^3$
160	344.3	38.7	234.1	1.60
		44.7	275.5	1.89
		47.7	296.2	2.00
		58.7	372.0	2.58
		73.7	475.5	3.21
		85.7	558.2	3.86
		96.7	634.0	4.23
		108.7	716.8	4.93
		125.2 .	830.5	$(5.49)^3$
				continued

¹Original data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water and butane were equilibrated in a cell at high pressure and constant temperature. A sample of the aqueous solution was passed into a low pressure Orsat gas buret for gas release under controlled conditions of temperature and pressure. At the pressure used (usually < 200 mm mercury) Henry's law, and the ideal gas law were assumed to describe the solubility, and gas volumetric properties, respectively. From a material balance as well as the vapor pressure and volume of water in the gas buret, the butane content of the original aqueous sample was calculated. Details in (1,2).

Data also reported for the threephase system.

SOURCE AND PURITY OF MATERIALS:

- 1. Phillips Petroleum Co. Certified purity of 99.9 mol per cent.
- 2. Distilled and deaerated.

ESTIMATED ERROR:

 $\delta P/P = 0.01$ (compiler) $\delta x_1/x_1 = 0.05$ (authors)

REFERENCES:

- Azarnoosh, A.; McKetta, J.J.
 Pet. Ref. <u>1958</u>, 37, 275.
- Wehe, A.H.; McKetta, J.J.
 Anal. Chem. <u>1961</u>, 33, 291.

²Calculated by compiler using vapor pressure data given by authors.

³Average of several determinations made at pressure of appearance of second liquid phase.

COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8] (2) Water; H₂O; [7732-18-5] VARIABLES: T/K: 310.9-410.9 P/kPa: 129.3-3044 ORIGINAL MEASUREMENTS: Le Breton, J.G.; McKetta, J.J. Hydroc. Proc. Pet. Ref. 1964, 43, 136-138. PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t¹/ºF	T 2 / K	Total Pressure ¹ /psia	Partial Pressure ² <i>P/</i> kPa	Mol Fraction $/10^5x_1$
220	377.6	68.7	355.1	2.24
		82.7	451.7	2.81
		102.7	589.6	3.84
		119.7	706.8	4.49
		126.7	755.0	4.84
		140.7	851.6	5.39
		147.7	899.8	6.32
		180.7	1127	7.24
		212.7	1348	8.02
		227.7	1451	8.26
		259.7	1672	(8.76) ³
280	410.9	89.7	279.2	2.19
		129.7	550.0	4.23
		164.7	796.3	6.29
		194.7	1003	7.64
		226.7	1224	9.17
		264.7	1486	11.01
		299.7	1727	12.26
		329.7	1934	13.31
		360.7	2148	14.40
		401.7	2430	15.70
		430.7	2630	16.415
		450.7	2768	16.86
		490.7	3044	$(17.71)^3$
				continued

¹Original data.

Data were also reported for the system involving two liquid (butane-rich, water-rich) phases.

 $^{^{2}\}text{Calculated}$ by compiler using vapor pressures of water given by authors.

³Average of two or more determinations made at the pressure of the appearance of the second liquid phase.

COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8] (2) Water; H₂O; [7732-18-5] VARIABLES: T/K: 310.9-410.9 P/kPa: 129.3-3044 ORIGINAL MEASUREMENTS: Le Breton, J.G.; McKetta, J.J. Hydroc. Proc. Pet. Ref. 1964, 43, 136-138. VRIABLES: VARIABLES: VARIABL

EXPERIMENTAL VALUES: (concluded)

Smoothed values were presented by authors as follows:

Fotal Pressure ¹ /psıa	T/K	Partial Pressure ² P ₁ /kPa	Mol Fraction 1 /10 5x_1
(0.9492) ³	310.9		
20	(100°F)	131.3	1.75
40	,	269.2	3.45
52.2		353.4	(4.40) 4
$(4.741)^3$	344.3		(1110)
20	(160°F)	105.2	0.75
40	, ,	243.1	1.60
60		381.9	2.55
80		518.9	3.45
100		656.8	4.40
125.2		830.5	(5.50) 4
$(17.186)^3$	377.6		(2121)
20	(220°F)	19.4	0.15
40		157.3	1.00
60		295.2	1.85
80		433.1	2.75
100		571.0	3.60
200		1260	7.65
259		1672	(9.10) 4
$(49.203)^3$	410.9		•
80	(280°F)	212.3	1.60
100		350.2	2.70
200		1040	9.70
300		1729	12.25
400		2419	15.65
490.7		3044	(17.80) 4

¹Original smoothed values.

²Calculated by compiler using authors' vapor pressure for water.

³Authors' vapor pressure for water.

[&]quot;Incidence of two liquid phases.

COMPONENTS: (1) Butane; C₄H₁₀; [106-97-8]

(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Danneil, A.; Todheide, K., and

Franck, E.U.

Chem. Ing-Tech. 1967, 13, 816-821.

VARIABLES:

T/K: 628.15, 637.15

P/MPa: 25.5-112.5

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t¹/°C	T/K	Pressure 1 P/bar	Pressure ² P/MPa	Mol Fraction in liquid/x ₁	n Butane: 1 in vapour/y
355	628.15	255	25.5	0.025	0.124
		295	29.5	0.048	0.105
		510	51.0	0.055	_
		520	52.0	_	0.188
		590	59.0	0.043	0.287
		725	72.5	0.036	_
		735	73.5	-	0.356
364	637.15	690	69.0	0.077	0.256
		830	83.0	0.041	0.318
		1090	109.0	-	0.417
		1125	112.5	0.041	-

¹Original data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static bomb with magnetically operated stirrer. Pressure measured with Bourdon gauge. Temperature measured with NiCr-Ni thermocouple. Samples of vapour and liquid analysed by stripping out hydrocarbon with carbon dioxide and estimating volumetrically. Water estimated gravimetrically.

SOURCE AND PURITY OF MATERIALS:

- Purity specified as 95.5 mol per cent.
- 2. Triply distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.7$; $\delta P/bar = \pm 1$ %

 $\delta x_1 = 0.005; \ \delta y_1 = 0.012 \ (authors)$

REFERENCES:

²Total pressure calculated by compiler.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Butane; C ₄ H ₁₀ ; [106-97-8]	Reamer, H. H.; Sage, B. H.; Lacey, W. N.		
(2) Water; H ₂ O; [7732-18-5]	Ind. Eng. Chem. 1952, 44, 609-615.		
VARIABLES:	PREPARED BY:		
T/K: 310.9-410.9 P/MPa: 0.355-3.735	W. Hayduk; C.L. Young		

		Total Gas Partial		11	Mole fractions		
T/K T/°F	Pressure p/psi	Pressure P/MPa	10 ⁵ x _{C4H10}	x'C4H10	^у С ₄ Н ₁₀		
310.9	100	52.45	0.355	6.2	0.9995	0.9833	
344.3	160	125.4	0.832	8.7	0.9979	0.9662	
377.6	220	259.3	1.669	14.0	0.9915	0.9459	
410.9	280	590.9	3.735	22.0	0.9732	0.9292	

a Mole fraction in water-rich liquid layer.

These data are at the limit of the three-phase region; at slightly lower pressures there are only two phases, gas and water.

Mole fraction of water rather than those of butane were given in the original.

Total pressure given in psia; gas partial pressure calculated in \mbox{MPa} by compilers.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Static equilibrium cell. Pressure measured with pressure balance and temperature measured with platinum resistance thermometer. Mixture confined to cell, the volume of which could be varied by mercury injection or withdrawal. Equilibrium established and samples withdrawn at constant pressure. Water content of sample determined by absorption in calcium chloride. Butane estimated volumetrically. Additional three-phase data in source and ref. (1) but no additional gas solubility data.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta P/MPa = \pm 0.007$; $\delta x_{C_4H_{10}} = \pm 5\%$, $\delta x_{C_4H_{10}}$, $\delta y_{C_4H_{10}} = \pm 1\%$ (estimated by compilers).

REFERENCES:

 Reamer, H. H.; Olds, R. H.; Sage, B. H.; Lacey, W. N. Ind. Eng. Chem. 1944, 36, 381.

b Mole fraction in hydrocarbon-rich liquid layer.